

**Examiner's Statement and Reasons for Allowance**

**Examiner's Statement and Amendment**

The after-final amendment to the claims filed on 5/5/10 is acknowledged and has been entered.

The rejection of claims 1-31 and 34 under 35 USC 112, second paragraph, is withdrawn in view of the amendment.

The rejection of claims 1-31 and 34 under 35 USC 112, first paragraph, is withdrawn in view of applicant's argument presented on page 9 of the response.

The Terminal Disclaimer (TD) filed 5/5/10 has been approved.

The rejection of claims 1-31 and 34 under the judicially created doctrine of obviousness-type double patenting is withdrawn in view of the TD.

Claims 1-31 and 34 are allowed with the following examiner's amendment.

An examiner's amendment to the record appears below. Should the changes and/or additions be unacceptable to applicant, an amendment may be filed as provided by 37 CFR 1.312. To ensure consideration of such an amendment, it MUST be submitted no later than the payment of the issue fee.

**In the claims:**

Cancel claim 32-33, which are drawn to unrelated inventions for reasons set forth in the previous Office action mailed 7/31/06. Note that the claims were nonelected, without traverse, in the response filed 12/29/06.

**Reasons for Allowance**

The following is an examiner's statement of reasons for allowance:

The prior art does not teach or suggest the claimed method: A computer-based method of generating 3-D structural models of complex formation between a query and a target macromolecule comprising a) providing a structural model of a query ligand and a structural model of a target macromolecule, wherein the structural model of the query ligand is based on data from X-ray crystallography or NMR spectroscopy, and the structural model of the target macromolecule is based on data from X-ray crystallography; b) identifying a substructure of the query ligand; c) identifying comparison ligands in a set of 3-D structural models that each share an identical substructure with the query ligand, wherein each 3-D structural model comprises a comparison ligand and a comparison macromolecule, and wherein the comparison macromolecule has structural features homologous to structural features of the target macromolecule of 20% or greater nucleic acid and/or amino acid homology; d) mapping spatial relationships between the substructure atoms of the query ligand and a comparison ligand identified in c) such that corresponding atoms are identified; e) assigning atomic coordinates to the corresponding atoms of the query ligand; f) generating and displaying one or more output models, each model comprising a 3-D structural model of the query ligand substructure and the target macromolecule, wherein the 3-D model of the query ligand substructure comprises the atomic coordinates of the query ligand from step e).

Any comments considered necessary by applicant must be submitted no later than the payment of the issue fee and, to avoid processing delays, should preferably accompany the issue fee. Such submissions should be clearly labeled "Comments on Statement of Reasons for Allowance."

Art Unit: 1631

**Inquiries**

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Shubo (Joe) Zhou, whose telephone number is 571-272-0724. The examiner can normally be reached Monday-Friday from 8 A.M. to 4 P.M.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Marjorie Moran, can be reached on 571-272-0720. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

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